CONTENTS

Thematic Issue on Time-Dependent Methods for Quantum Dynamics
Editor: K.C. Kulander

Forward xi

Preface xii

Contents xiii

Berman, M. and R. Kosloff
Time-dependent solution of the Liouville–von Neumann equation: non-dissipative evolution 1

Zimmerer, P., M. Zimmermann, N. Grün and W. Scheid
Trajectory method for the time-dependent Schrödinger and Thomas–Fermi equations 21

Zhang, J.Z.H.
Multichannel quantum wave-packet propagation in the interaction picture: application to gas–surface scattering 28

Billing, G.D.
Basis set independent methods in time-dependent dynamics 38

Sun, Y., D.J. Kouri, D.W. Schwenke and D.G. Truhlar
Time-dependent wave-packet algorithm for inelastic molecule–molecule scattering 51

Bottcher, C., G.J. Bottrell and M.R. Strayer
Time-dependent Hartree–Fock studies of atomic collisions 63

Shi, S. and H. Rabitz
Optimal control of bond selectivity in unimolecular reactions 71

Richardson, J.L.
Visualizing quantum scattering on the CM-2 supercomputer 84

DeVries, P.L.
The time evolution of the hydrogen wavefunction in intense laser fields 95

Mowrey, R.C. and D.J. Kouri
Inelastic molecule-corrugated surface scattering using the close-coupling wave-packet method 100

Horbatsch, M.
A semiclassical independent electron model for ion–atom collisions 115

Balint-Kurti, G.G., R.N. Dixon, C.C. Marston and A.J. Mulholland
The calculation of product quantum state distributions and partial cross-sections in time-dependent molecular collision and photodissociation theory 126

Iung, C. and C. Leforestier
Exact time evolution methods for large bound systems 135

Jackson, B.
Time-dependent mean-field approach to molecule–surface scattering at finite temperatures 154

Kwong, N.H., K.J. Schaudt and J.D. Garcia
Solution of quantum evolution equations by finite-difference 171

Umar, A.S. and M.R. Strayer
Numerical methods for nuclear mean-field dynamics 179

Mickens, R.E.
Novel explicit finite-difference schemes for time-dependent Schrödinger equations 203

Balakrishnan, N. and N. Sathyamurthy
Time-dependent wave-packet methods for the calculation of collinear atom–diatom exchange reaction probabilities 209

Jolicard, G. and J. Humbert
Stationary and time-dependent wave-operator formulation in molecular dynamics 216

Engel, V.
Excitation of molecules with ultrashort laser pulses: exact time-dependent quantum calculations 228

Kotler, Z., E. Neria and A. Nitzan
Multiconfiguration time-dependent self-consistent field approximations in the numerical solution of quantum dynamical problems 243

Pernot, P., W.A. Lester Jr. and Ch. Cerjan
Quantum time-dependent treatment of molecular collisions: scattering of He by $H_2(B^1(\Sigma_u^+)$ 259

Faisal, F.H.M. and P. Scanzano
Solution of the initial value-problem in laser–atom interaction: a variational Fourier transform method 265

Spina, A. and R.T. Skodje
The phase-space hydrodynamic model for the quantum standard map 279

Shafer, K.J., N.H. Kwong and J.D. Garcia
Development of B-spline techniques for dynamic ion–metal interaction theories 306

Mancini, R.C., D.P. Kilcrease, L.A. Woltz and C.F. Hooper Jr.
Calculation aspects of the Stark line broadening of multi-electron ions in plasmas 314

McCurdy, C.W. and C.K. Stroud
Eliminating wave-packet reflection from grid boundaries using complex coordinate contours 323

Srivastava, D. and D.A. Micha
Complex-time path-integration with time-dependent Hamiltionans for extended molecular systems 331

Lüdde, H.J. and R.M. Dreizler
Microscopic optical potentials for time-dependent quantum systems 345

Tiszauer, D.H. and K.C. Kulander
Computation methods employed in the self-consistent time-dependent, Hartree–Fock calculation for a reactive molecular collision 351

Berger, J.F., M. Girod and D. Gogny
Time-dependent quantum collective dynamics applied to nuclear fission 365

Gauss, J. and E.J. Heller
A time-dependent semiclassical wave-packet method using a fast Fourier transform (FFT) algorithm 375

Makri, N.
Feynman path integration in quantum dynamics 389

Thirumalai, D. and B.J. Berne
Methods for simulating time correlation functions in quantum systems 415

Schafer, K.J.
The energy analysis of time-dependent numerical wave functions 427

Dateo, C.E., V. Engel, R. Almeida and H. Metiu
Numerical solutions of the time-dependent Schrödinger equation in spherical coordinates by Fourier transform methods 435

Heather, R.W.
An asymptotic wavefunction splitting procedure for propagating spatially extended wavefunctions: application to intense field photodissociation of H_2^+ 446

Neuhauser, D., M. Baer, R.S. Judson and D.J. Kouri
The application of time-dependent wavepacket methods to reactive scattering 460

Chu, S.-I. and T.-F. Jiang
Nonperturbative methods for the study of multiphoton dynamics in intense periodic and multicolor laser fields 482

Webster, F., P.J. Rossky and R.A. Friesner
Nonadiabatic processes in condensed matter: semi-classical theory and implementation 494

Kulander, K.C. and T.N. Rescigno
Effective potentials for time-dependent calculations of multiphoton processes in atoms 523

Cerjan, C. and K.C. Kulander
Efficient time propagation for finite-difference representations of the time-dependent Schrödinger equation 529

Lin, F.J. and J.T. Muckerman
Solution of the time-dependent Schrödinger equation employing a basis of explicit discrete-coordinate eigenfunctions: spherical and azimuthal symmetry, adiabaticity, and multiphoton excitation of a rotating Morse oscillator 537

Besprozvannaya, A. and D.J. Tannor
Fast sine/cosine transform for periodic functions with reflection symmetry 569

Author index to volume 63 579

Subject index to volume 63 583

Program index to volume 63 584